

REPRESENTING AGGREGATE SIZE DISTRIBUTIONS AS MODIFIED LOG-NORMAL DISTRIBUTIONS

by

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SUMMARY:

A wider range of field-sampled, aggregate size distributions can be described more accurately using 3- or 4-parameter, modified, log-normal functions compared to the traditional, 2-parameter, log-normal function. Comparisons of the standard and modified log-normal forms are presented, as well as a discussion of selected computational approaches for determination of function coefficients.

KEYWORDS:

aggregate size distribution, log-normal distribution, curve-fitting, frequency distribution

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ABSTRACT*

Historically, the 2-parameter log-normal distribution has been the method of choice when describing soil aggregate size distributions and generally provides a good description. However, the assumptions regarding the upper and lower extremes of the 2-parameter log-normal ogive can limit the applicability of the standard log-normal distribution. Many tillage-induced aggregate size distributions cannot be adequately represented by a 2-parameter log-normal ogive. Two 3-parameter and one 4-parameter log-normal ogives are presented that can more accurately describe a wider range of field-sampled aggregate size distributions. Computational techniques for determining values for the coefficients of these modified log-normal functions are also discussed¹.

INTRODUCTION

The size distribution of soil aggregates affects many facets of agriculture from wind erosion susceptibility (Chepil, 1950a, 1953) to seedbed suitability (Hadas and Russo, 1974; Schneider and Gupta, 1985). Gardner (1956) demonstrated that the 2-parameter log-normal distribution provided a good description of the aggregate size distribution of many soils. Kemper and Chepil (1956) concurred with Gardner, extolling the virtue of summarizing aggregate size distribution data with only the two parameters, geometric mean diameter, x_g , and geometric standard deviation, σ_g . Unfortunately, they did not recommend this method for general use because of the extensive work required to adequately sieve field samples and the computational effort required to determine the parameters. This led to the adoption of many less meaningful measures of aggregate size distribution. For this reason, Hagen et al. (1987) presented a computerized iteration procedure that required only two sieves to determine the parameters for a standard, 2-parameter, log-normal ogive to characterize aggregate size distribution of dry soil. The one caveat that Gardner mentioned is that any field-sampled, aggregate size distribution will exhibit some deviation at the extremes from a standard log-normal ogive. Hagen et al. (1987), also realizing this limitation, suggested the possibility of using 3- or 4-parameter log-normal forms if the tails of the distributions are important to the application of the data.

The Wind Erosion Prediction System (WEPS), presently being developed by the Agricultural Research Service, USDA (Hagen, 1991), requires the dry aggregate size distribution to be accurately represented on a daily basis within the model. A standard log-normal ogive implies that the smallest aggregate size is zero and the largest size is infinite. Agricultural soils have upper and lower size limits that account for deviations of aggregate size distributions from log-normality. For these reasons, a more complete method of representing aggregate size distribution was desired for WEPS.

Kottler (1950a), Irani (1959), and Irani and Callis (1963) examined situations that arose when data conforming to log-normality had all sizes greater than or less than a specified size (or both) removed from the data set. The modified data sets were actually similar to many of the data sets typically presented as being log-normal distributions. In these "non-ideal" cases, physical constraints limit the "growth" or "breakdown" process, and, therefore, are not truly log-normal. The "limited growth" and "limited breakdown" processes were represented by a log-normal ogive by using simple transformations that satisfied the new boundary conditions. Because dry aggregate size distributions have some limiting maximum and minimum sizes, modified log-normal ogives should more accurately represent these distributions. The purpose of this paper is to describe the procedures required to determine parameters of the modified log-normal ogive and present methods for computing their values. Comparisons between the standard and modified log-normal ogives were made using actual aggregate size distributions determined from sieved field samples.

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¹ Code employing the computational methods discussed are available upon request by sending a DOS compatible disk to the author.

THEORY

Particle sizes, such as soil aggregate sizes, are frequently found empirically to fit the log-normal distribution function. Suppose that x is the quantity being measured (e.g., aggregate size). It will be found to be distributed with a density function, $p(x)$, where $p(x)dx$ is the probability that a measured value will fall within the range $[x, x+dx]$.

If x is described by a log-normal distribution, then $y=\ln(x)$ has a normal distribution $n(y)$,

$$n(y) = \frac{1}{\sigma\sqrt{2\pi}} \exp \left[-\frac{(y-\mu)^2}{2\sigma^2} \right] \quad -\infty < y < +\infty \quad (1)$$

in which the parameters μ and σ^2 are respectively, the mean and the variance of the y values. Because $n(y)$ is symmetric about the mean, μ is also the median of the normal distribution (on the average, half the y values will be greater than μ and half will be less).

Because $p(x)$ and $n(y)$ describe the same phenomenon, the probability of obtaining values in corresponding dy and dx intervals must be equal, i.e., $p(x)dx = n(y)dy$. Thus, the log-normal distribution $p(x)$ is given by Eq. [2].

$$p(x) = n(y) \frac{dy}{dx} = \frac{1}{x\sqrt{2\pi}\sigma^2} \exp \left[-\frac{(\ln(x)-\mu)^2}{2\sigma^2} \right] \quad 0 < x < +\infty \quad (2)$$

The average value of x is defined as:

$$x_{av} \equiv \int_0^{\infty} x p(x) dx = \int_{-\infty}^{\infty} e^y n(y) dy \quad (3)$$

Because $y=\ln(x)$, we have,

$$x_m = e^\mu \quad (4)$$

Substituting Eq. [2] and [4] into Eq. [3] and integrating, we have:

$$x_{av} = e^{(\mu+\sigma^2/2)} \quad (5)$$

For a log-normal distribution, σ^2 is always larger than zero; thus, based on Eq. [4] and [5], the log-normal distribution can be fully described by the median size, x_m , and the mean size, x_{av} . In other words, from the observed mean and median, values for μ and σ^2 of the approximating log-normal distribution can be estimated as shown in Eq. [6] and Eq. [7].

$$\mu = \ln(x_m) \quad (6)$$

$$\sigma^2 = 2[\ln(x_{av}) - \mu] = 2[\ln(x_{av}) - \ln(x_m)] \quad (7)$$

However, most log-normal distributions are expressed in terms of the geometric mean, x_g , and geometric standard deviation, σ_g , which are defined as $\sigma_g = e^\sigma$ and $x_g = e^\mu$, respectively. Substituting x_g and σ_g into Eq. [2], $p(x)$ can be expressed in terms of x_g and σ_g as shown in Eq. [8].

$$p(x) = \frac{1}{x\sqrt{2\pi} \ln(\sigma_g)} \exp \left[-\frac{1}{2} \left(\frac{\ln(x/x_g)}{\ln(\sigma_g)} \right)^2 \right] \quad 0 < x < +\infty \quad (8)$$

For many analyses, it is often useful to express the measured distribution in terms of the *cumulative probability distribution*, $F(x)$, which is the probability (or frequency) that a measured value will be less than or equal to x . If $t = \ln(x/x_g)/\ln(\sigma_g)$, then for the log-normal distribution, this cumulative distribution function of x is given by:

$$F(x) \equiv \int_0^x p(x) dx = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^t e^{-t^2/2} dt = \frac{1}{2} + \frac{1}{2} \operatorname{erf} \left(\frac{t}{\sqrt{2}} \right) = \frac{1}{2} + \frac{1}{2} \operatorname{erf} \left(\frac{\ln(x) - \ln(x_g)}{\sqrt{2} \ln(\sigma_g)} \right) \quad (9)$$

Thus, the probability of x , $P(\% \leq x)$ and $P(\% \geq x)$, in terms of percent, can be calculated as:

$$P(\% \leq x) = 100 F(x) = 50 + 50 \operatorname{erf} \left(\frac{\ln(x) - \ln(x_g)}{\sqrt{2} \ln(\sigma_g)} \right) \quad (10)$$

$$P(\% \geq x) = 100 - P(\% \leq x)$$

Kottler (1950a) treated particle size distributions from a kinetic point of view. He discussed the concept of "limited growth" in which most phenomena of normal growth have a rate that increases only during an initial period and afterwards decreases gradually. He introduces a lower limit, x_o (corresponding to the absolute minimum particle size), which must be greater than zero and an upper limit, x_∞ (corresponding to the absolute maximum size obtained), which must be less than infinity. By using the transformation, $\hat{x} = (x - x_o)(x_\infty - x_o)/(x_\infty - x)$ in which x is in the range of $[x_o, x_\infty]$, where $0 \leq x_o < x_\infty < +\infty$, a more general 4-parameter log-normal case, Eq. [11], can be introduced.

$$p(\hat{x}) = \frac{1}{\hat{x}\sqrt{2\pi} \ln(\hat{\sigma}_g)} \exp \left[-\frac{1}{2} \left(\frac{\ln(\hat{x}/\hat{x}_g)}{\ln(\hat{\sigma}_g)} \right)^2 \right] \quad 0 < \hat{x} < +\infty \quad (11)$$

The corresponding cumulative distribution function, in terms of percent, are:

$$\hat{P}(\% \leq x) = 50 \left[1 + \operatorname{erf} \left\{ \frac{\ln \left(\frac{(x - x_o)(x_\infty - x_o)}{(x_\infty - x)\hat{x}_g} \right)}{\sqrt{2} \ln(\hat{\sigma}_g)} \right\} \right] \quad (12)$$

$$\hat{P}(\% \geq x) = 100 - \hat{P}(\% \leq x)$$

\hat{x}_g and $\hat{\sigma}_g$ can be determined from computational procedures discussed later. To obtain the x_g value from \hat{x}_g , simply perform the reverse transformation operation of \hat{x} as shown in Eq. [13]. Note that x_g is the 50% value, x_{50} , and represents the "middle" of the distribution.

$$x_g = x_{50} = \frac{\hat{x}_g x_\infty + x_o x_\infty - x_o^2}{x_\infty - x_o + \hat{x}_g} \quad (13)$$

To obtain the σ_g value from $\hat{\sigma}_g$, compute the arithmetic average of the \hat{x} values, \hat{x}_{av} ,

$$\hat{x}_{av} = \hat{x}_g e^{\frac{1}{2} \ln^2(\hat{\sigma}_g)} \quad (14)$$

to obtain x_{av} , perform the transformation as shown in Eq. [15] on \hat{x}_{av} ,

$$x_{av} = \frac{\hat{x}_{av}x_{\infty} + x_o x_{\infty} - x_o^2}{x_{\infty} - x_o + \hat{x}_{av}} \quad (15)$$

and then compute σ_g as a function of x_{av} and x_g as shown in Eq. [16].

$$\sigma_g = e^{\frac{1}{2} \ln^2 \left(\frac{x_{av}}{x_g} \right)} \quad (16)$$

If $x_o=0$ and $x_{\infty} \rightarrow \infty$, this general case, Eq. [11], will reduce to the simple or standard, 2-parameter, log-normal distribution, Eq. [2] and its corresponding cumulative distribution function, Eq. [10]. The two, 3-parameter, modified, log-normal forms are derived when either the lower value, x_o , equals zero or the upper value, x_{∞} , approaches infinity. All of these log-normal forms are summarized in Table 1.

COMPUTATIONAL PROCEDURES

Two methods of computing the parameters for the four forms of the log-normal ogives discussed here were implemented. One method uses a direct computational scheme, and the second employs a nonlinear optimization technique to determine the "best" parameters based on the the cumulative distribution curve.

The direct computational scheme outlined by Allen (1981) and Campbell (1985) assumes that the data are log-normally distributed and works best when the sieve cuts are sized according to a geometric progression. It requires an estimate of the minimum size, x_{min} , and the maximum size, x_{max} , (to determine the geometric means, $x_{g(0)}$ and $x_{g(n)}$, of the smallest and largest sieve cuts respectively). Also, if a modified log-normal form is being used, $x_{min} < x_o < x_{g(0)}$, and $x_{g(n)} < x_{\infty} < x_{max}$.

The limitations of this method are that: a) an estimate of the geometric means of the smallest and largest sieve cuts must be made; b) the limits of the distribution, x_o and x_{∞} , must be known (or their ranges known if an optimization technique is employed to determine them); and c) if the smallest and/or largest sieve cuts have no material in them for a particular distribution, they must be removed from the computations if the limiting parameters, x_o and/or x_{∞} , need to fall within those size ranges. The benefit of the direct computational scheme is that it is very fast and does not require any iterative procedures, making it ideal for applications where speed is critical.

For the direct computational procedure, the geometric mean diameter, \hat{x}_g , and geometric standard deviation, $\hat{\sigma}_g$, are:

$$\hat{x}_g = e^a \quad \text{and} \quad \hat{\sigma}_g = e^b$$

where:

$$a = \sum_{i=1}^n [m_i \ln(\hat{x}_{g(i)})], \quad b = \left[\sum_{i=1}^n [m_i \ln^2(\hat{x}_{g(i)})] - a^2 \right]^{\frac{1}{2}} \quad (17)$$

i = sieve cut
 $\hat{x}_{g(i)} = \sqrt{\hat{x}_{i(lower)} \hat{x}_{i(upper)}} = \text{geometric mean within sieve cut } i$
 n = total number of sieves cuts
 m_i = mass fraction of sieve cut i

The second method uses a constrained optimization procedure presented by Box (1963) to estimate the parameters of the cumulative frequency curve for any of the selected log-normal forms (Eq. [11]). The function used to determine the "best fit" was the weighted sum of the squared residuals due to error (SSE) as shown in Eq. [18].

$$SSE = \sum_{i=1}^n w_i (\hat{y}_i - y_i)^2$$

where:

$$\begin{aligned} i &= \text{data value} \\ n &= \text{total number of data values} \\ x_i &= \text{sieve size for data value } i \\ y_i &= \text{actual } \hat{P}(\% \leq x_i) \\ \hat{y}_i &= \text{estimate of } \hat{P}(\% \leq x_i) \\ w_i &= \text{weighting factor for data value } i \end{aligned} \quad (18)$$

The actual and predicted probabilities less than (or greater than) the sieved sizes were used as the y values. A weighting factor of 1 was used. Other weighting schemes may be used depending upon the region of interest. Kottler (1950b) suggested that "fitting" log-normal data should generally employ a probability weighting factor if the 50% point is of greatest interest.

The limitation of this method is that it is an iterative procedure and, therefore, may not be appropriate for use in applications where speed is critical. Nevertheless, it will determine the "best fit" without the limitations and assumptions required of the direct computation procedure. It does need estimates of the upper and lower ranges for each of the parameters being determined. These can be set broadly enough to encompass all expected size distributions. Narrower ranges, if known, will allow the optimization procedure to "close in" on the solution faster, but are not strictly required. By setting the upper and lower ranges equally for a particular parameter, then the optimization routine would effectively force the "best fit" model to have the desired value for that parameter.

DISCUSSION

Often, the standard log-normal form will overpredict the amount of small material and underpredict the amount of large material when used to classify field aggregate size distributions, because the distributions have a lower size limit greater than zero and an upper finite size limit. Modified log-normal forms are means of more accurately describing field-sampled aggregate size distributions, including their upper and lower tails.

Many tillage-induced aggregate size distributions are influenced by the amount and size of the largest aggregates in the field prior to tillage. Wagner and Ding (1992) showed that disk tillage operations primarily break down large aggregates (greater than 50 mm) when they are present, but act on a wide range of aggregate sizes when large aggregates do not exist. Therefore, the resulting post-tillage, maximum, aggregate size, as well as aggregate size

distribution, is dependent upon the pre-tillage aggregate size distribution. Future advances in modeling aggregate breakdown by tillage operations will necessarily require accurate representation of the pre-tillage aggregate size distribution, including the upper size segment.

The complete aggregate size distribution provides useful information about wind erosion processes. For example:

1. Given different aggregate size distributions with the same percentage of erodible aggregates (less than 0.84 mm), Chepil (1950b) showed that aggregate size distributions with smaller non-erodible aggregates resulted in more rapid surface armoring and, thus, a less erodible fraction available for direct emission. In other words, small non-erodible aggregates provide more surface cover and shelter for the erodible aggregates than do large non-erodible aggregates. Therefore, with a complete aggregate size distribution, we should be able to determine the amount of "shelter" provided by non-erodible aggregates.
2. Given a complete aggregate size distribution and a shelter angle distribution and assuming that the smallest aggregates are residing in the most sheltered areas, we can:
 - a. compute the fraction of soil surface where friction velocity is above saltation threshold,
 - b. compute the volume of particles available for emission (Hagen, 1991), and
 - c. potentially compute the fraction of PM-10 (sub 10 μm size particles) present for direct emission (PM-10 has health and regulatory implications).
3. With a complete aggregate size distribution, we can also determine the effect of sorting by wind erosion. Size ranges for saltation, suspension, and emission materials change with windspeed and surface roughness. Therefore, these components could then be viewed together with the surface aggregate size distribution.

Figures 1 and 2 both illustrate how 3 and 4-parameter modified log-normal functions more accurately represent actual aggregate size distributions. This is verified by the respective R^2 values (Table 2) for each of the log-normal forms in the figures. Figure 1 is a post-tillage aggregate size distribution from a Kimo silty clay loam (clayey over loamy, montmorillonitic, mesic Fluvaquent Montmorillonitic) in which a very high percentage of large aggregates was formed. The chisel-shank spacing, however, probably helped limit the size of the aggregates formed and is reflected in the sharp rise in the cumulative distribution curve at the upper end. The upper size limit, x_{∞} , was determined to have a value of 101.6 mm, as shown in Table 2, for the 3-parameter log-normal estimate of the aggregate size distribution in figure 1.

Figure 2 is an aggregate size distribution from a Reading silt loam (fine-silty, mixed, mesic Typic Argiudoll) that had the smaller fraction sieved into additional size classes to more accurately determine the form of the lower tail of the distribution. Notice that this distribution also reflects a large amount of big aggregates that causes the cumulative distribution to deviate from a straight line. The 4-parameter log-normal form fit this distribution very well and determined the lower limit, x_0 , to be 0.17 mm and the upper limit, x_{∞} , to be 45.71 mm (Table 2).

The standard, 2-parameter, log-normal distribution is completely described by x_g and σ_g . By definition, the geometric mean, x_g , for the 2-parameter log-normal function directly provides the size at which 50% is greater and 50% is less than its value. The geometric standard deviation, σ_g , is defined as the ratio of the size at 84.13% probability to the size at 50% probability (or the size at 50% probability to the size at 15.87% probability) and indicates the dispersion or range of sizes for a 2-parameter log-normal function.

The addition of new parameters for the modified log-normal functions allow more accurate descriptions of typical size distributions, but makes comparisons of such size distributions more difficult. Note that the \hat{x}_g and $\hat{\sigma}_g$ terms (Table 1) for the three modified log-normal functions are not directly comparable with each other or with x_g and σ_g terms from the standard log-normal function. Both \hat{x}_g and $\hat{\sigma}_g$ are defined in terms of the transformation variable, \hat{x} , and are functions of the x_0 and x_{∞} parameters. Thus, \hat{x}_g and $\hat{\sigma}_g$ parameters represent the physical relationships

mentioned above, but they apply to the transformed variable, \hat{x} , and not to the original variable, x , for the modified log-normal functions. This will usually cause misleading comparisons between different distributions based solely on the modified log-normal parameters. This can be seen by inspecting the parameter values provided in Table 2.

Ropp (1985) discussed this problem along with the tendency of many researchers to assume normality or even log-normality and then present only the fraction of interest. He suggested that the most effective method for displaying aggregate size distributions is to use a log-normal probability method. Because no one parameter or group of parameters can be defined for use when presenting and discussing all size distribution information, visual presentation of the data and summarization of the parameters describing the complete distribution are requisite, especially when using one of the modified log-normal forms.

SUMMARY AND CONCLUSIONS

Modified forms of the standard log-normal functions can be used effectively to describe a broader range of aggregate size distributions determined from sieving field samples. The modified methods assume that either a limiting, non-zero, minimum size or a finite maximum size exists (or both), which is normally true for aggregate size distributions. Therefore, the modified log-normal forms usually can represent a size distribution more accurately, especially at the tails, than a standard log-normal function. A more accurate description of aggregate size distributions helps depict wind erosion processes in greater detail and allows models such as WEPS to better simulate them.

Two methods for computing the parameters of all four log-normal functions were presented. One was a direct computation method, which is useful for applications where computation speed is a factor. The second method uses a non-linear optimization technique, which will find the "best fit" parameter values more precisely, but requires more computational overhead.

Data should be collected and relationships formed between tillage operations, soil types, and soil conditions for models such as WEPS to reliably predict tillage-induced aggregate size distribution. Investigations into the relationships between the maximum, tillage-induced, aggregate size and the tillage tool should be explored. Field samples also should be studied to determine if correlations exist between the minimum aggregate sizes found and the amount of PM-10 material produced under various conditions and operations.

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Table 1. Standard and modified log-normal forms.

Case	Log-Normal Form	Constraints	Parameters
I	standard 2-parameter	$0 \leq x < \infty$	x_g, σ_g
II	modified 3-parameter	$0 \leq x \leq x_\infty < \infty$	$\hat{x}_g, \hat{\sigma}_g, x_\infty$
III	modified 3-parameter	$0 < x_o \leq x < \infty$	$\hat{x}_g, \hat{\sigma}_g, x_o$
IV	modified 4-parameter	$0 < x_o \leq x \leq x_\infty < \infty$	$\hat{x}_g, \hat{\sigma}_g, x_o, x_\infty$

Table 2. Standard and modified log-normal coefficients for two aggregate size distributions.

Soil	Log-Normal Form	x_{50}	σ_g	R^2	\hat{x}_g	$\hat{\sigma}_g$	x_o	x_∞
Kimo	2-parameter	16.13	5.47	.98	16.13	5.47	-	-
silty clay loam	3-parameter	28.66	4.74	.99	39.88	15.89	-	101.60
Reading	2-parameter	2.46	8.90	.95	2.46	8.90	-	-
silt loam	4-parameter	3.47	9.31	.99	3.73	22.66	0.017	45.71

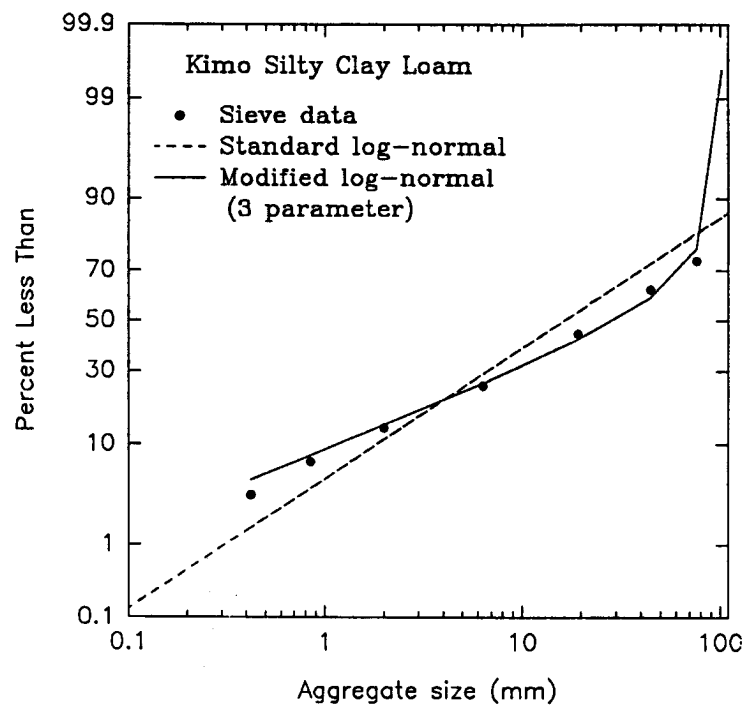


Figure 1. ASD sample from a Kimo silty clay loam.

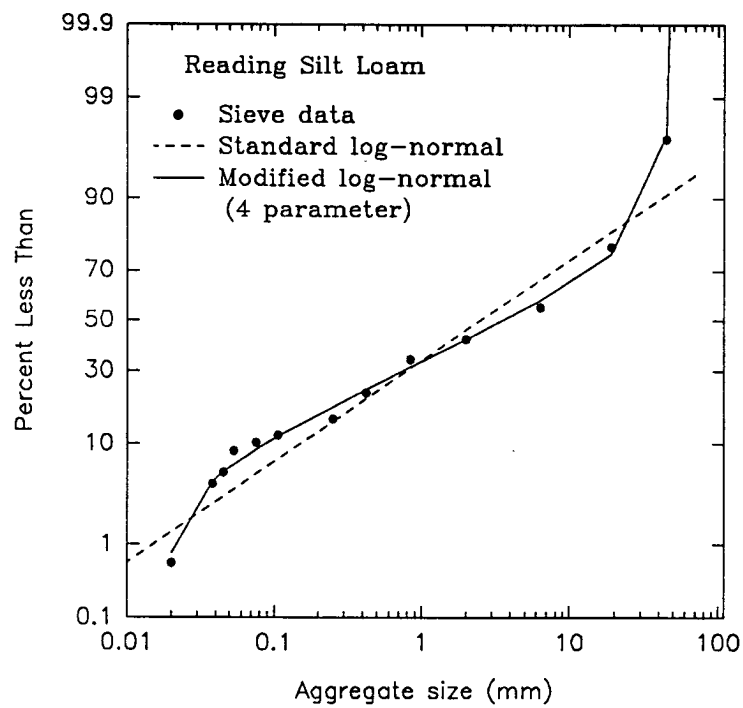


Figure 2. ASD sample from a Reading silt loam.